

10/579 222

INVENTOR SEARCH

=> file reg  
FILE 'REGISTRY' ENTERED AT 17:53:14 ON 20 AUG 2007  
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STRUCTURE FILE UPDATES: 19 AUG 2007 HIGHEST RN 944998-48-5  
DICTIONARY FILE UPDATES: 19 AUG 2007 HIGHEST RN 944998-48-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

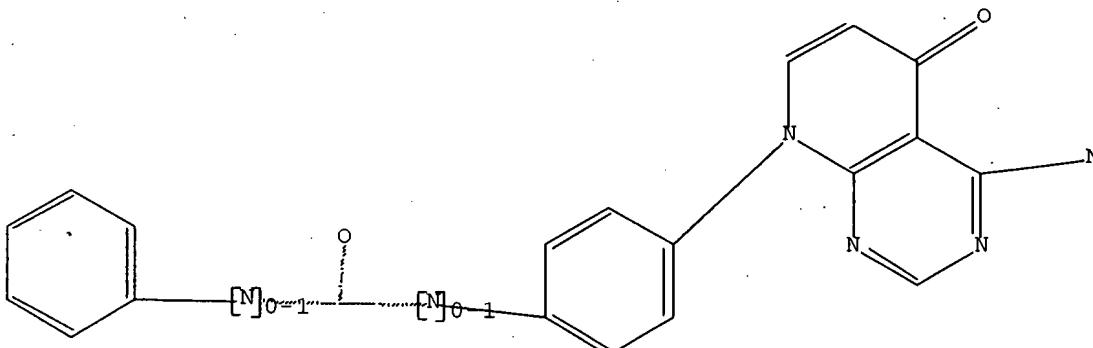
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d stat que 17  
L5 STR

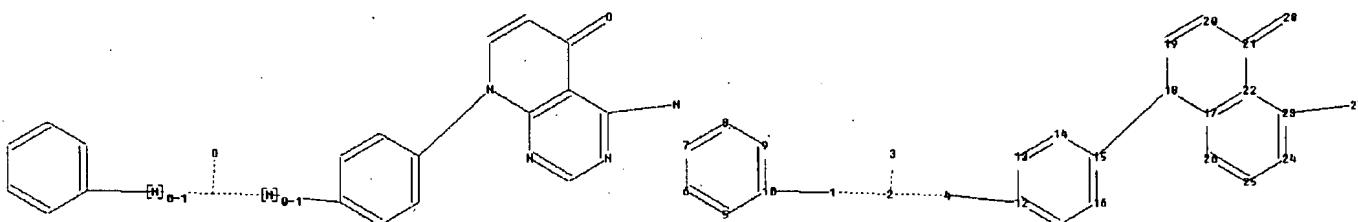


Structure attributes must be viewed using STN Express query preparation.  
L7 66 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 1965 ITERATIONS  
SEARCH TIME: 00.00.01

66 ANSWERS

Uploading jai222.str



chain nodes :

1 2 3 4 27 28

ring nodes :

5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26

chain bonds :

1-2 1-10 2-3 2-4 4-12 15-18 21-28 23-27

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18

17-22 17-26 18-19 19-20 20-21 21-22 22-23 23-24 24-25 25-26

exact/norm bonds :

1-2 1-10 2-3 2-4 4-12 15-18 17-18 18-19 19-20 20-21 21-22 21-28 23-27

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-22

17-26 22-23 23-24 24-25 25-26

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom

=> file hcaplus

FILE 'HCAPLUS' ENTERED AT 17:54:37 ON 20 AUG 2007

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FILE COVERS 1907 - 20 Aug 2007 VOL 147 ISS 9

FILE LAST UPDATED: 19 Aug 2007 (20070819/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos 131

L20 83 SEA FILE=HCAPLUS ABB=ON PLU=ON HOELZEMANN G?/AU

L21 13 SEA FILE=HCAPLUS ABB=ON PLU=ON CRASSIER H?/AU

L22 200 SEA FILE=HCAPLUS ABB=ON PLU=ON ACKERMANN K?/AU

L23	30 SEA FILE=HCAPLUS ABB=ON	PLU=ON	STAEHLE W?/AU
L24	285 SEA FILE=HCAPLUS ABB=ON	PLU=ON	JONCZYK A?/AU
L25	52 SEA FILE=HCAPLUS ABB=ON	PLU=ON	RAUTENBERG W?/AU
L26	21 SEA FILE=HCAPLUS ABB=ON	PLU=ON	MITJANS F?/AU
L27	12 SEA FILE=HCAPLUS ABB=ON	PLU=ON	ROSELL-VIVES E?/AU
L28	21 SEA FILE=HCAPLUS ABB=ON	PLU=ON	MITJANS F?/AU
L29	21 SEA FILE=HCAPLUS ABB=ON	PLU=ON	ADAN J?/AU
L30	110 SEA FILE=HCAPLUS ABB=ON	PLU=ON	SOLER R?/AU
L31	1 SEA FILE=HCAPLUS ABB=ON	PLU=ON	L20 AND L21 AND L22 AND L23 AND L24 AND L25 AND L26 AND L27 AND L28 AND L29 AND L30

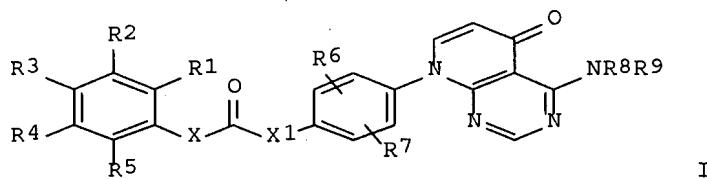
=> d ibib ed abs l31

L31 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2005:451380 HCAPLUS Full-text  
 DOCUMENT NUMBER: 142:482058  
 TITLE: Preparation of pyridopyrimidinones as inhibitors  
 of tyrosine and Raf kinases for treatment of  
 tumors.  
 INVENTOR(S): Hoelzemann, Guenter; Crassier,  
 Helene; Ackermann, Karl-August;  
 Staehle, Wolfgang; Jonczyk,  
 Alfred; Rautenberg, Wilfried;  
 Mitjans, Francesc; Rosell-Vives,  
 Elisabet; Adan, Jaume;  
 Soler, Riera Marta  
 PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany  
 SOURCE: PCT Int. Appl., 95 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
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WO 2005047283	A1	20050526	WO 2004-EP11549	200410 14		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	DE 10352979	A1	20050609	DE 2003-10352979	200311 13
AU 2004288727	A1	20050526	AU 2004-288727	200410 14		

CA 2545558	A1	20050526	CA 2004-2545558	
				200410
				14
EP 1682548	A1	20060726	EP 2004-790407	
				200410
				14
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2007510679	T	20070426	JP 2006-538680	
				200410
				14
US 2007099910	A1	20070503	US 2007-579222	
				200701
				09
PRIORITY APPLN. INFO.:			DE 2003-10352979	A
				200311
				13
			WO 2004-EP11549	W
				200410
				14

OTHER SOURCE(S): MARPAT 142:482058  
 ED Entered STN: 27 May 2005  
 GI



AB Title compds. [I; R1-R5 = H, A, OH, OA, alkenyl, alkynyl, NO<sub>2</sub>, NH<sub>2</sub>, NHA, NA<sub>2</sub>, halo, cyano, CO<sub>2</sub>H, COA, CO<sub>2</sub>A, O-Het, etc.; pairs of R1-R5 = OCH<sub>2</sub>CH<sub>2</sub>, OCH<sub>2</sub>O, OCH<sub>2</sub>CH<sub>2</sub>O, OCF<sub>2</sub>O, OCA<sub>2</sub>O; R6, R7 = H, A halo, OA, cyano; R8, R9 = H, alkyl optionally interrupted by O, N; Het = mono- or bicyclic (unsatd.) (aromatic) heterocycl; A = (fluoro- and/or chloro-substituted) alkyl; X, X1 = NH, null], were prepared as inhibitors of tyrosine and Raf kinases (no data). Thus, 4-amino-8-(4-aminophenyl)-8H-pyrido[2,3-d]pyrimidin-5-one (preparation given) was stirred overnight with 2-fluoro-5-trifluoromethylphenyl isocyanate and Et<sub>3</sub>N in CH<sub>2</sub>Cl<sub>2</sub> to give 1-[4-(4-amino-5-oxo-5H-pyrido[2,3-d]pyrimidin-8-yl)phenyl]-3-(2-fluoro-5-trifluoromethylphenyl)urea.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

STRUCTURE SEARCH

=> file reg  
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STRUCTURE FILE UPDATES: 19 AUG 2007 HIGHEST RN 944998-48-5  
DICTIONARY FILE UPDATES: 19 AUG 2007 HIGHEST RN 944998-48-5

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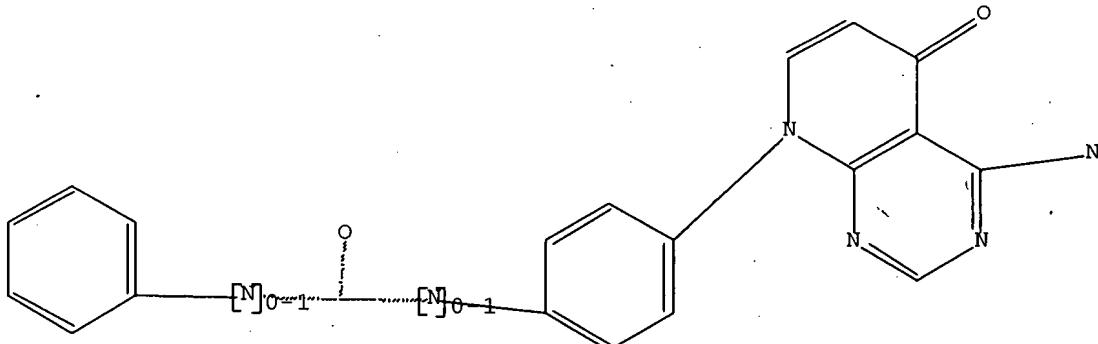
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d stat que l7  
L5 STR

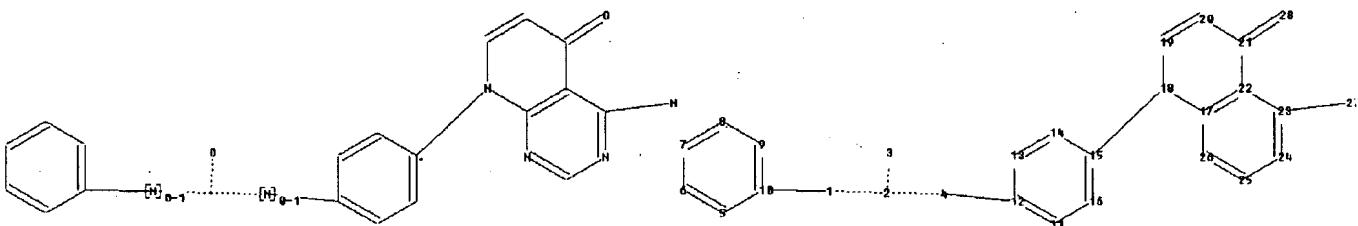


Structure attributes must be viewed using STN Express query preparation.  
L7 66 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 1965 ITERATIONS  
SEARCH TIME: 00.00.01

66 ANSWERS

Uploading jai222.str



chain nodes :

main menu:

ring nodes :

Fring Nodes .

chain bonds :

chain bonds

ring bonds : C=C1C=CC=C1

Final Scores : 5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 1

17-22 17-26 18-1

exact/norm bonds :

1=2 1=10 2=3 2=

normalized bonds : [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) [11](#) [12](#) [13](#) [14](#) [15](#) [16](#) [17](#) [18](#) [19](#) [20](#) [21](#) [22](#) [23](#) [24](#) [25](#)

normalized bonds :

Match level : **1. M1**   **2. M2**   **3. M3**   **4. M4**   **5. M5**   **6. M6**   **7. M7**   **8. M8**   **9. M9**   **10. M10**

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

=> file hcaplus

FILE 'HCAPLUS' ENTERED AT 17:55:35 ON 20 AUG 2007

FILE #CA74553 ENTERED AT 17:35:39 ON 20 AUG 2007  
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FILE COVERS 1907 - 20 Aug 2007 VOL 147 ISS 9  
FILE LAST UPDATED: 19 Aug 2007 (20070819/ED)

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'OBT' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos 18

L5 STR  
L7 66 SEA FILE=REGISTRY SSS FUL L5  
L8 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

=> file casreact  
FILE 'CASREACT' ENTERED AT 17:55:48 ON 20 AUG 2007  
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FILE CONTENT:1840 - 18 Aug 2007 VOL 147 ISS 9

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\*\*\*\*\*  
\*  
\* CASREACT now has more than 12 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que nos 19  
L5 STR  
L7 66 SEA FILE=REGISTRY SSS FUL L5  
L9 0 SEA FILE=CASREACT ABB=ON PLU=ON L7

=> file marpat  
FILE 'MARPAT' ENTERED AT 17:56:07 ON 20 AUG 2007  
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FILE CONTENT: 1961-PRESENT VOL 147 ISS 7 (20070817/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 2007155779 05 JUL 2007  
DE 102005063244 28 JUN 2007  
EP 1801190 27 JUN 2007  
JP 2007173472 05 JUL 2007  
WO 2007076379 05 JUL 2007  
GB 2433499 27 JUN 2007  
FR 2895408 29 JUN 2007  
RU 2302407 10 JUL 2007

CA 2571093 16 JUN 2007

Expanded G-group definition display now available.

=> d que nos 118  
L5 STR  
L18 5 SEA FILE=MARPAT SSS FUL L5

=> file beilstein  
FILE 'BEILSTEIN' ENTERED AT 17:57:06 ON 20 AUG 2007  
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FILE LAST UPDATED ON June 25, 2007

FILE COVERS 1771 TO 2007.

\*\*\* FILE CONTAINS 10,004,722 SUBSTANCES \*\*\*

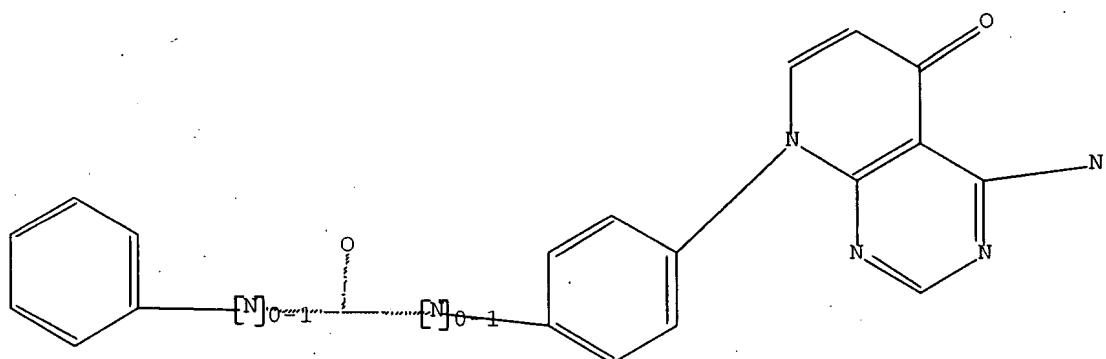
>>> PLEASE NOTE: Reaction Data and substance data are stored in  
separate documents and can not be searched together in one query.  
Reaction data for BEILSTEIN compounds may be displayed  
immediately with the display codes PRE (preparations) and REA  
(reactions). A substance answer set retrieved after the search  
for a chemical name, a compounds with available reaction  
information by combining with PRE/FA, REA/FA or more generally  
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link  
between a BEILSTEIN compound and belonging reactions. For mo  
detailed reaction searches BRNs can be searched as reaction  
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\*\*\*\*\*  
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\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE \*  
\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE, THESE \*  
\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. \*  
\* FOR PRICE INFORMATION SEE HELP COST \*  
\*\*\*\*\*

NEW  
\* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE  
SEARCHED, SELECTED AND TRANSFERRED.  
\* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,  
ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A  
COMPOUND AT A GLANCE.

=> d stat que 112  
L5 STR

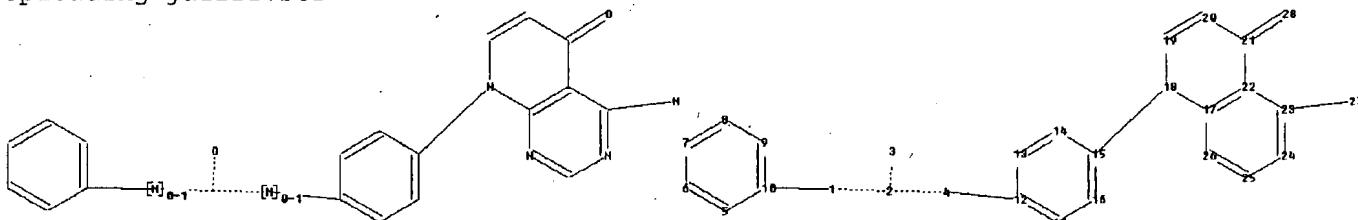


Structure attributes must be viewed using STN Express query preparation.  
L12 0 SEA FILE=BEILSTEIN SSS FUL L5

100.0% PROCESSED 442 ITERATIONS  
SEARCH TIME: 00.00.02

0 ANSWERS

Uploading jai222.str



chain nodes :

1 2 3 4 27 28

ring nodes :

5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26

chain bonds :

1-2 1-10 2-3 2-4 4-12 15-18 21-28 23-27

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18

17-22 17-26 18-19 19-20 20-21 21-22 22-23 23-24 24-25 25-26

exact/norm bonds :

1-2 1-10 2-3 2-4 4-12 15-18 17-18 18-19 19-20 20-21 21-22 21-28 23-27

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-22

17-26 22-23 23-24 24-25 25-26

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom

20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom

=> file hcplus marpat

FILE 'HCPLUS' ENTERED AT 17:57:23 ON 20 AUG 2007

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=> dup rem l16 l18  
PROCESSING COMPLETED FOR L16  
PROCESSING COMPLETED FOR L18  
L32 7 DUP REM L16 L18 (3 DUPLICATES REMOVED)  
ANSWERS '1-5' FROM FILE HCAPLUS  
ANSWERS '6-7' FROM FILE MARPAT

=> d que nos 132  
L5 STR  
L7 66 SEA FILE=REGISTRY SSS FUL L5  
L8 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L7  
L16 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 AND PY>2005  
L18 5 SEA FILE=MARPAT SSS FUL L5  
L32 7 DUP REM L16 L18 (3 DUPLICATES REMOVED)

=> s 132 not 131  
L33 6 L32 NOT L31

=> d ibib ed abs hitstr 1-4;d ibib abs qhit 5-6

L33 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2006:364321 HCAPLUS Full-text  
DOCUMENT NUMBER: 144:412515  
TITLE: Heterocyclic substituted bisarylurea derivatives  
as kinase inhibitors and their preparation,  
pharmaceutical compositions, and use for  
treatment of diseases mediated or propagated by  
kinases  
INVENTOR(S): Stieber, Frank; Jonczyk, Alfred; Hoelzemann,  
Guenter; Buchstaller, Hans-Peter; Burgdorf, Lars  
Thore; Rautenberg, Wilfried; Greiner, Hartmut  
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany  
SOURCE: PCT Int. Appl., 232 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2006040056	A1	20060420	WO 2005-EP10744	200510 06

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CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI,  
GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM,  
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,  
MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,

RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
 RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU,  
 IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR,  
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,  
 TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,  
 ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

AU 2005293839 A1 20060420 AU 2005-293839

200510  
06

CA 2584185 A1 20060420 CA 2005-2584185

200510  
06

EP 1799669 A1 20070627 EP 2005-789864

200510  
06

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU,  
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 TR

IN 2007KN01680 A 20070727 IN 2007-KN1680

200705  
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PRIORITY APPLN. INFO.: EP 2004-24369

A  
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EP 2005-16845

A  
200508  
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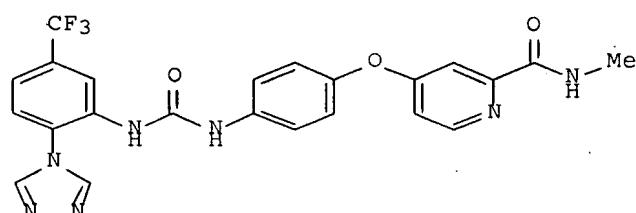
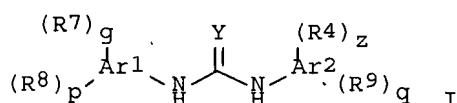
WO 2005-EP10744

W  
200510  
06

OTHER SOURCE(S): MARPAT 144:412515

ED Entered STN: 21 Apr 2006

GI



AB The invention relates to heterocyclic substituted bisarylurea derivs. of formula I, the use of the compds. of formula I as inhibitors of one or more kinases, the use of the compds. of formula I for the manufacture of a pharmaceutical composition and a method of treatment, comprising administering said pharmaceutical composition to a patient. Compds. of formula I wherein R4 is (X-Ar3) $\alpha$ - (R10)10; Ar1, Ar2, and Ar3 are independently 5- to 14-membered unsatd. or aromatic cyclic hydrocarbon, or 2- to 10-membered unsatd. or aromatic heterocyclic residue, preferably 1 to 5 heteroatoms selected from N, O, and S;  $\alpha$  is 0, 1, or 2; r, z, and p are independently 0, 1, 2, 3, 4 or 5; R7 is nitrogen containing heterocyclic moiety bound directly to Ar1 via a nitrogen atom, etc.; R8, R9, and R10 are independently H, (alkoxy)alkyl, alkenyl, C3-7 cycloalkyl, alkenylcycloalkyl, halo, CH<sub>2</sub>halo, CH(halo)2, C(halo)3, NO<sub>2</sub>, etc.; Y is O, S, NH and derivs., (un)substituted CHNO<sub>2</sub>, (un)substituted CHCN, or C(CN)2; g is 1, 2, or 3; q is 0, 1, 2, 3 or 4; and their pharmaceutically acceptable derivs., salts and solvates thereof are claimed in this invention. Example compound II was prepared by chlorination and esterification of pyridine-2-carboxylic acid to give Me 4-chloropyridine-2-carboxylate, which underwent amidation with methylamine to give 4-chloropyridine-2-carboxylic acid methylamide, which was reacted with 4-aminophenol; the resulting 4-(4-aminophenoxy)pyridine-2-carboxylic acid methylamine reacted with p-nitrophenyl chloroformate and 4-(2-amino-4-trifluoromethylphenyl)-1,2,4-triazole to give example compound II. All the invention compds. were evaluated for their activity as modulators and inhibitors of kinases. From the assay, it was determined that these compds. preferably inhibit VEGF-stimulated mitogenesis of human vascular endothelial cells in cultures with IC<sub>50</sub> values of 0.01-5.0  $\mu$ M.

IT 883881-42-3P 883881-43-4P 883881-48-9P

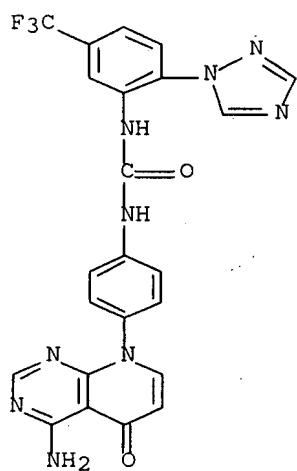
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heterocyclic substituted bisarylurea derivs. that are able to inhibit or modulate signaling of kinases useful for treatment of diseases mediated or propagated by kinases)

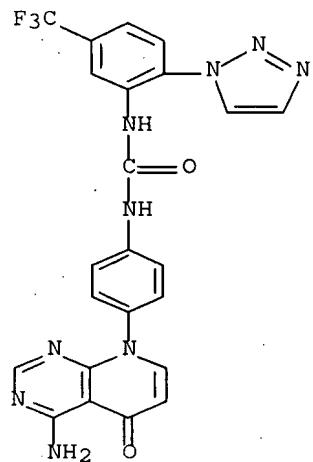
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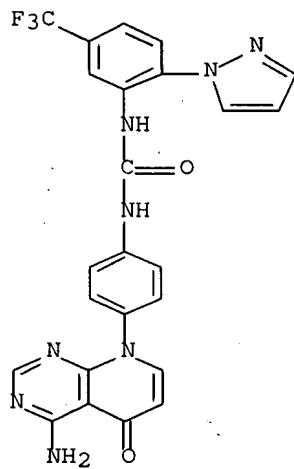
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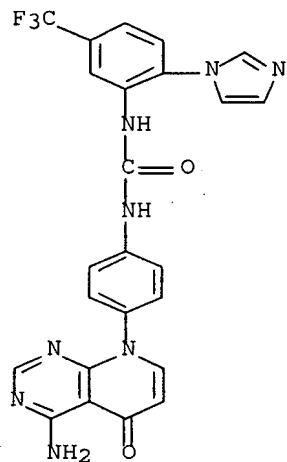
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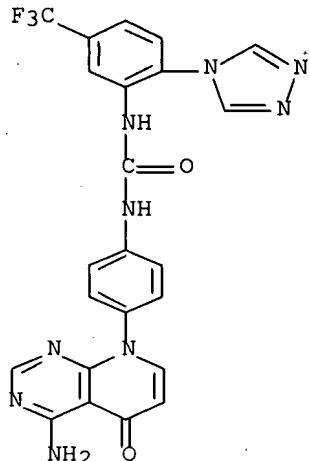
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RN 883881-57-0 HCPLUS

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REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2005:1103581 HCAPLUS Full-text

DOCUMENT NUMBER: 143:360132

TITLE: Methods for modulating glutamate receptors for treating neuropsychiatric disorders comprising the use of modulators of serum and glucocorticoid inducible kinases909

INVENTOR(S): Lang, Florian

PATENT ASSIGNEE(S): Merck Patent GmbH, Germany

SOURCE: PCT Int. Appl., 36 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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OTHER SOURCE(S): MARPAT 143:360132

ED Entered STN: 14 Oct 2005

AB The invention discloses modulation of the activity of serum and glucocorticoid inducible kinases to restore glutamate receptor activity. Also disclosed are methods and compds. useful for the detection and treatment of neuropsychiatric disorders.

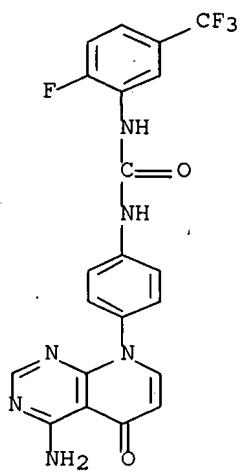
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(serum and glucocorticoid inducible kinase modulators for glutamate receptor modulation and treatment of neuropsychiatric disorders)

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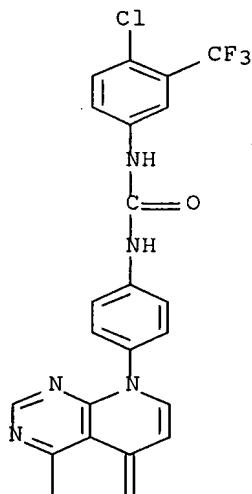
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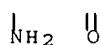
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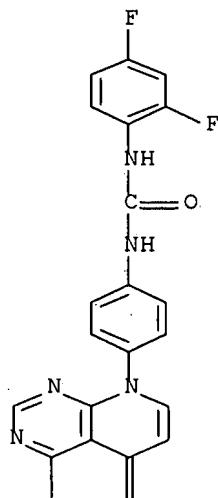
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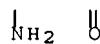
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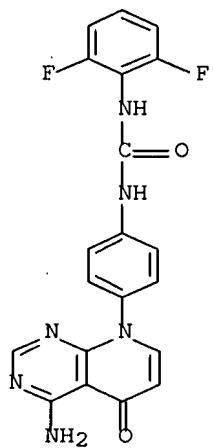


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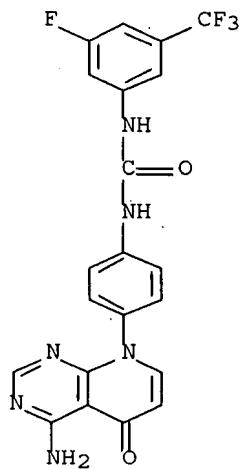
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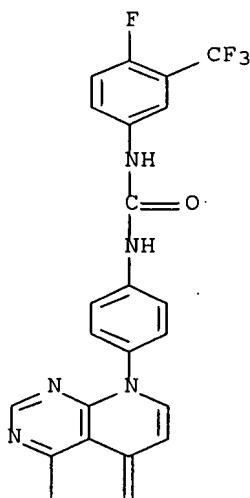
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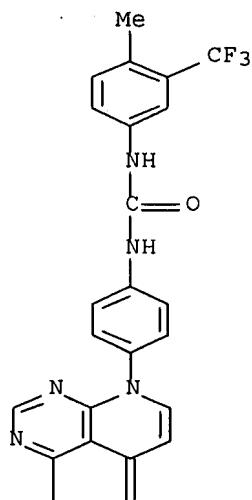
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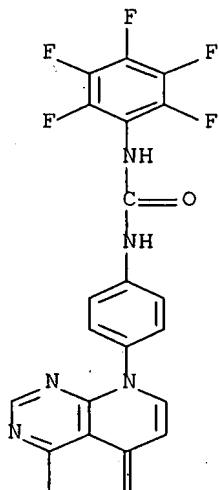
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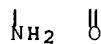
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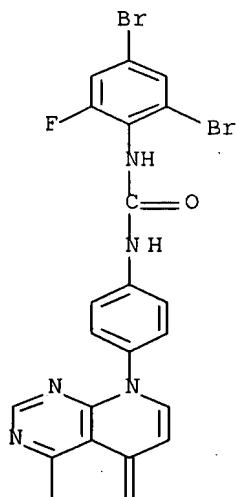
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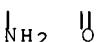
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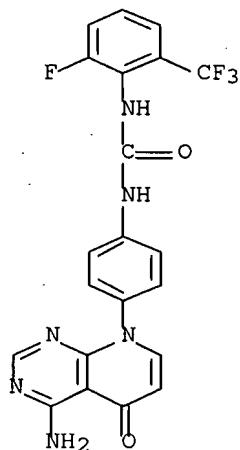


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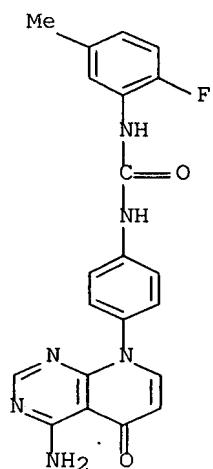
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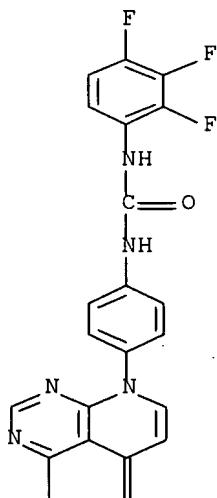
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CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(2,3,4-trifluorophenyl)- (9CI) (CA INDEX NAME)

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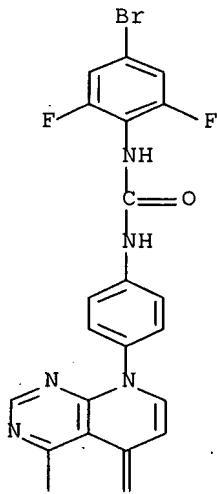
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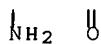


RN 852221-59-1 HCPLUS

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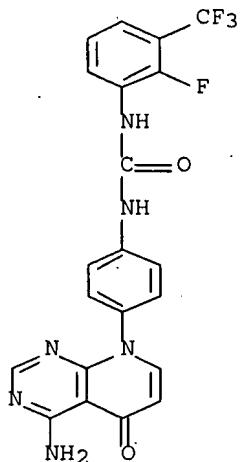
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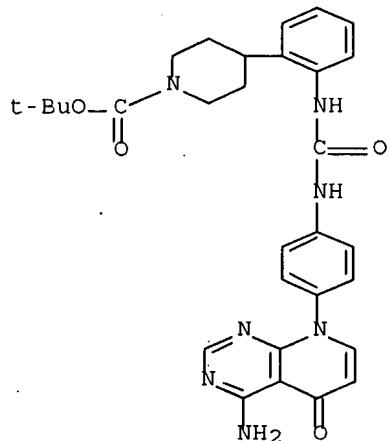
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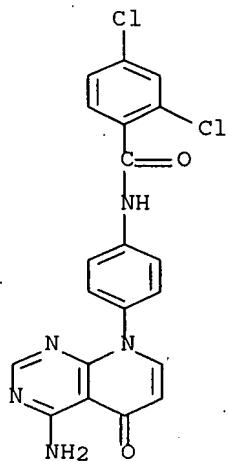
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CN 1-Piperidinecarboxylic acid, 4-[2-[[[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]amino]carbonyl]amino]phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



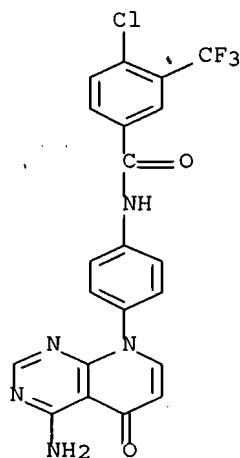
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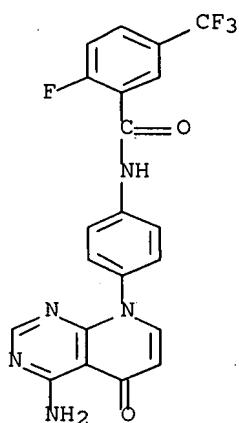
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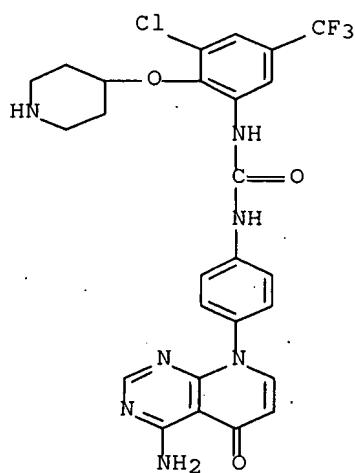
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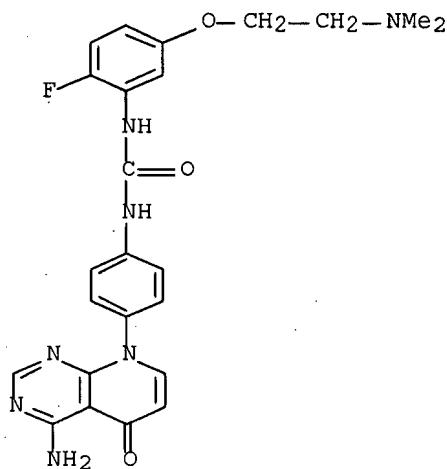
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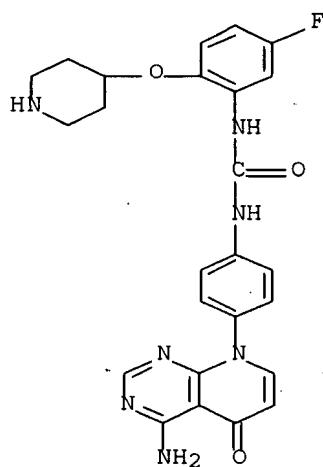
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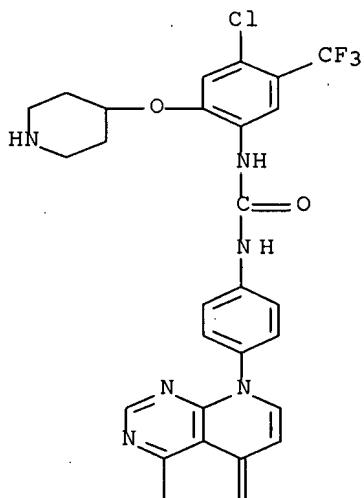
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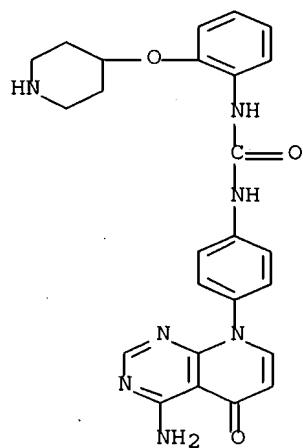


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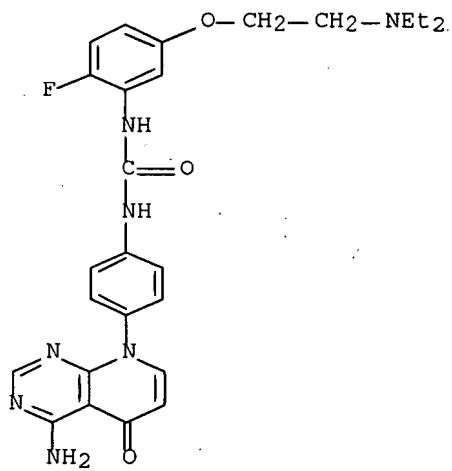
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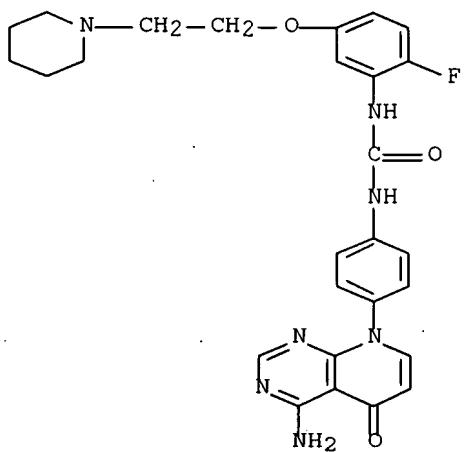
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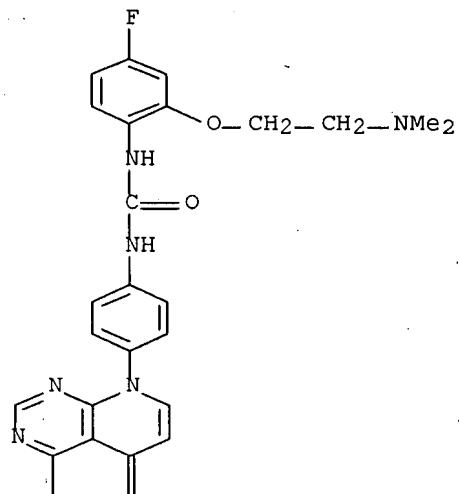
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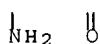
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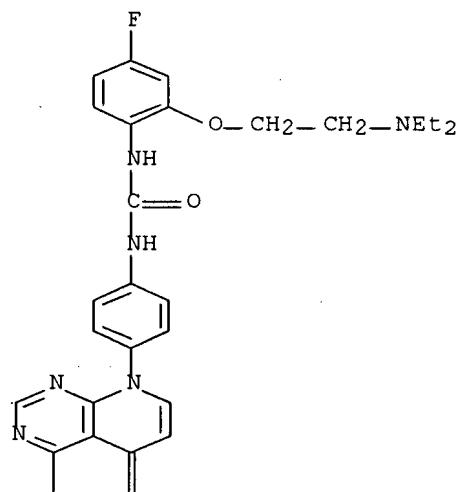
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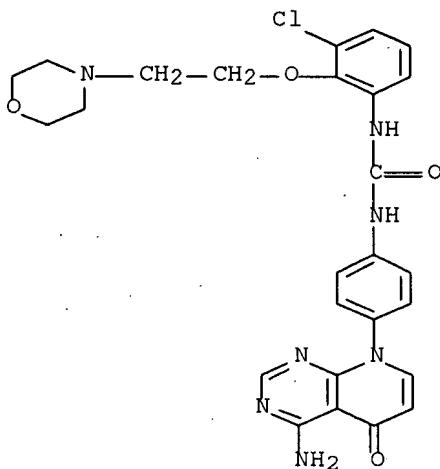
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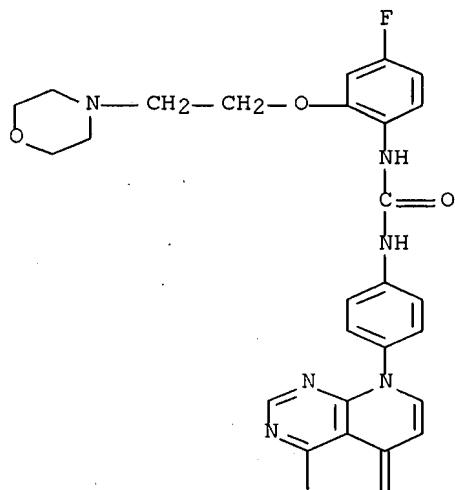
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RN 852221-90-0 HCAPLUS

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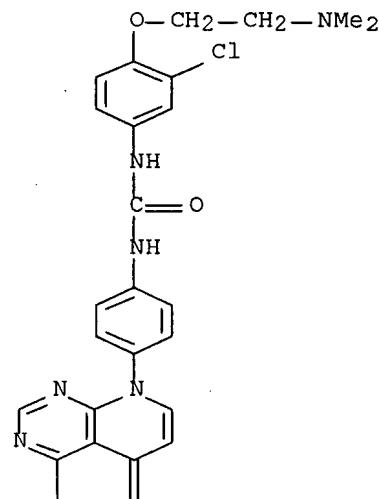
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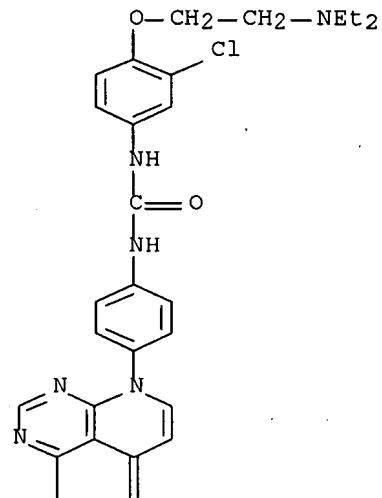
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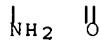
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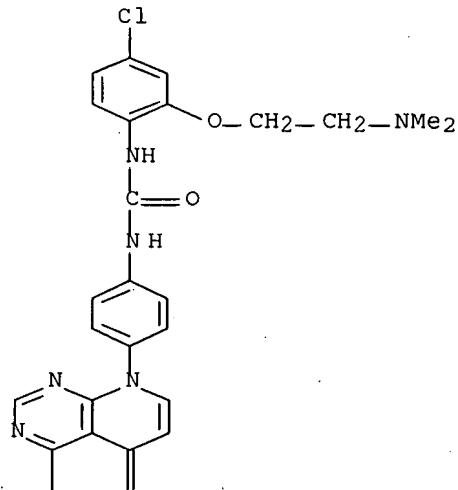
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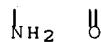
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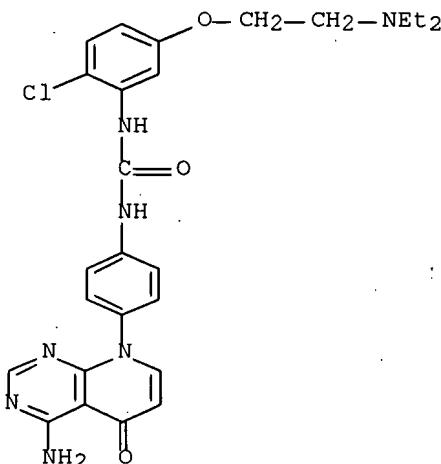


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REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN  
• ACCESSION NUMBER: 2005:1103556 HCAPLUS Full-text  
DOCUMENT NUMBER: 143:379867  
TITLE: Modulation of connective tissue growth factor activity for diagnosis and treatment of fibrosis  
INVENTOR(S): Lang, Florian  
PATENT ASSIGNEE(S): Merck Patent GmbH, Germany  
SOURCE: PCT Int. Appl., 26 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005094796 A3 20061228  
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GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,  
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ED Entered STN: 14 Oct 2005

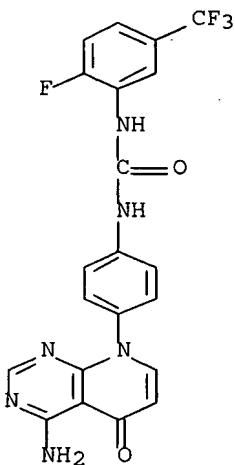
AB An increased expression of connective tissue growth factor strongly correlates with the presence and upregulation of the serum/glucocorticoid inducible kinase SGK1. Modulation of the of glucocorticoid inducible kinases, SGK1, SGK2, and SGK3 to restore connective tissue growth factor activity is described. Methods and acyl hydrazone and pyridopyrimidine compds. useful for the detection and treatment of fibroproliferative disorders are provided.

IT 852221-35-3 852221-37-5 852221-39-7  
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 852221-47-7 852221-49-9 852221-51-3  
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RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (acyl hydrazones and pyridopyrimidines as inhibitors of serum/glucocorticoid inducible kinases for diagnosis and treatment of fibrosis)

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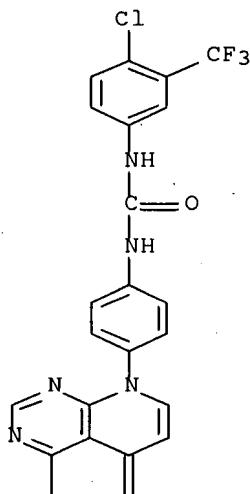
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RN 852221-37-5 HCPLUS

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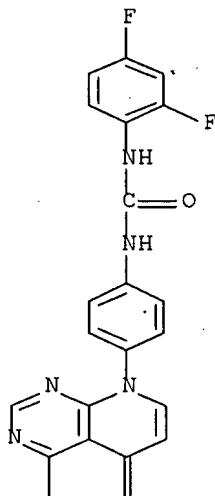


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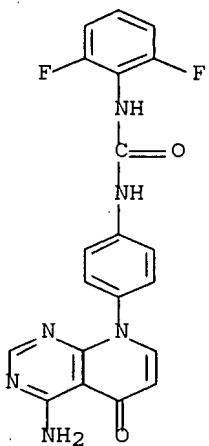


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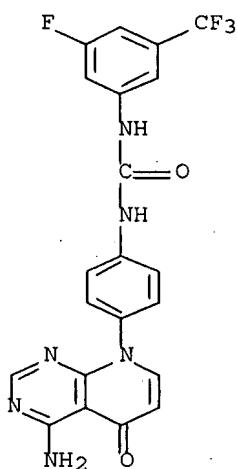
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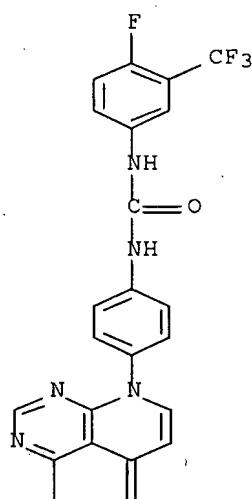
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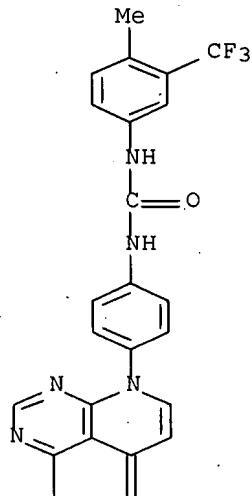
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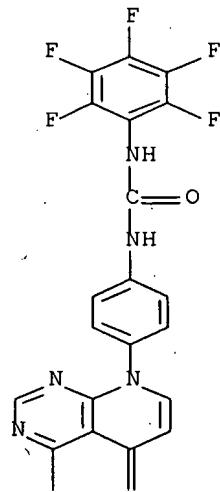
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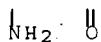
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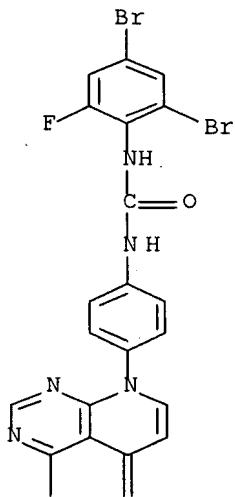
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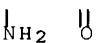
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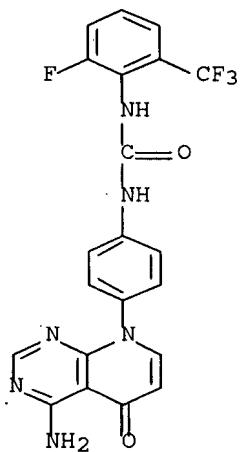


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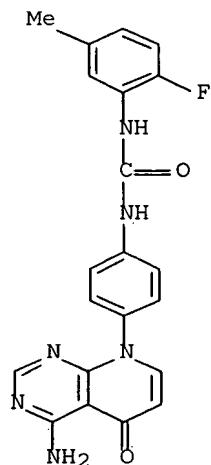
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RN 852221-55-7 HCAPLUS

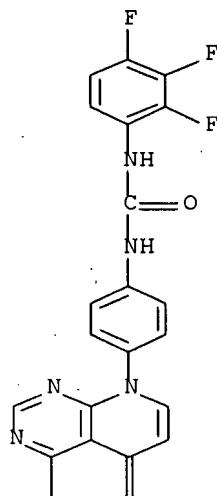
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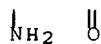
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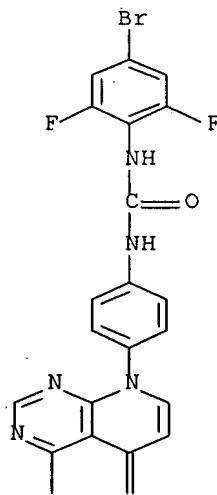
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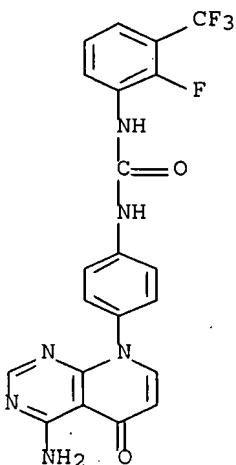
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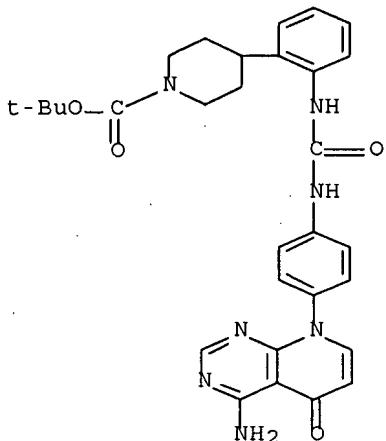
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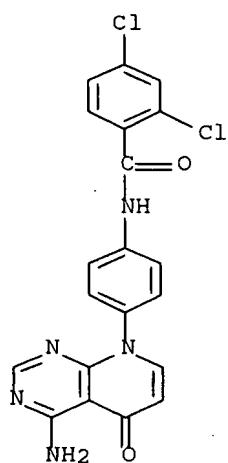
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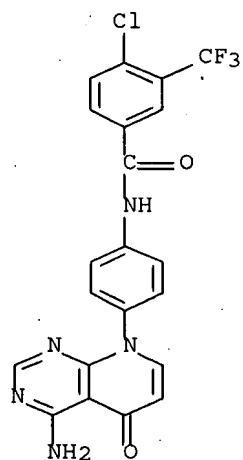
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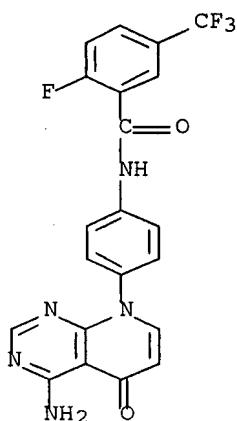
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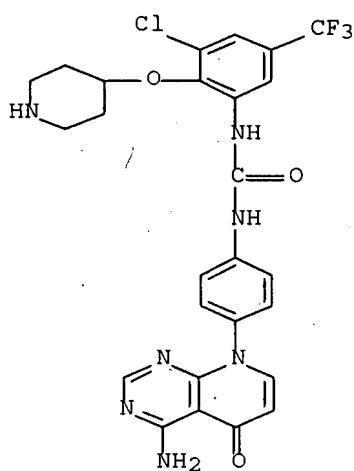
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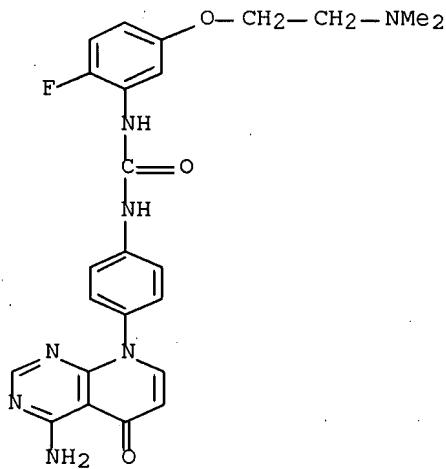
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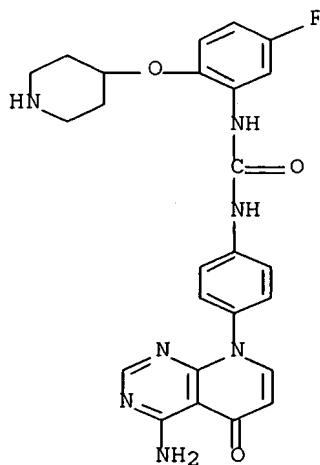
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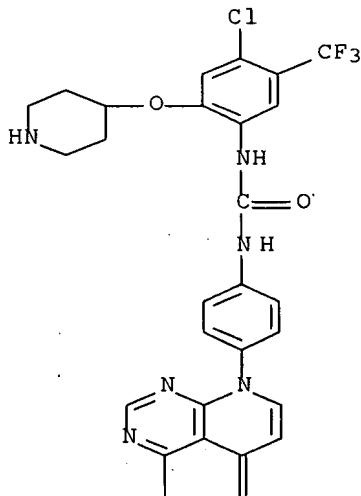
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RN 852221-76-2 HCPLUS

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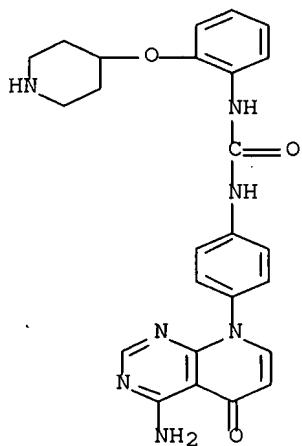


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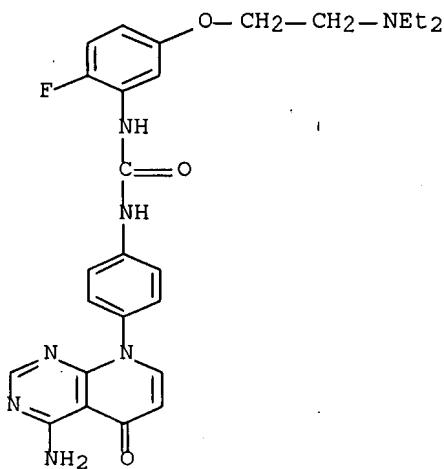
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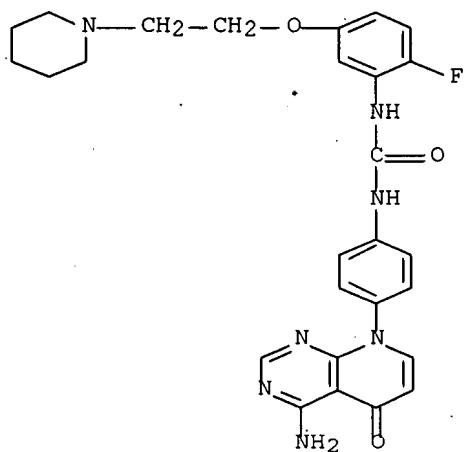
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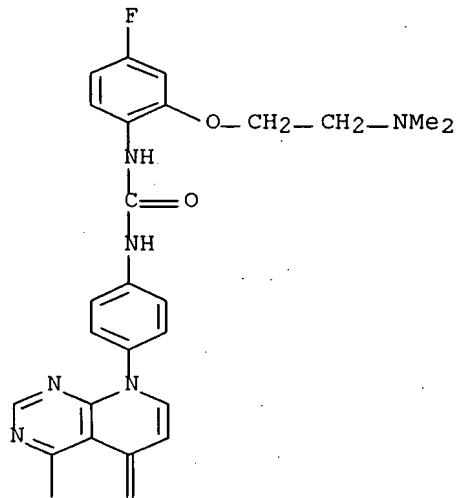
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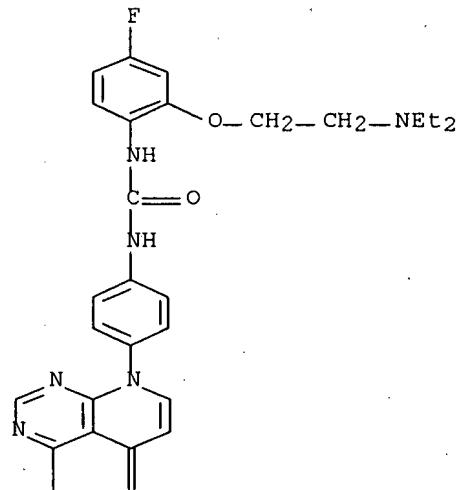
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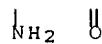
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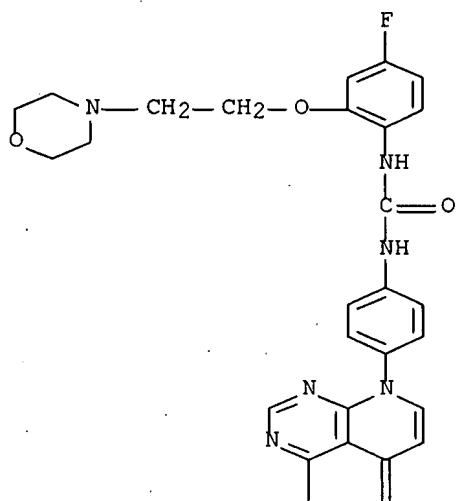
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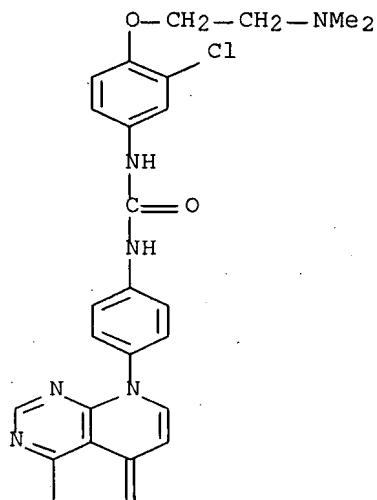
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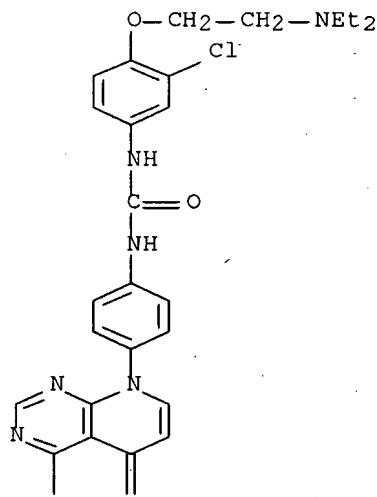
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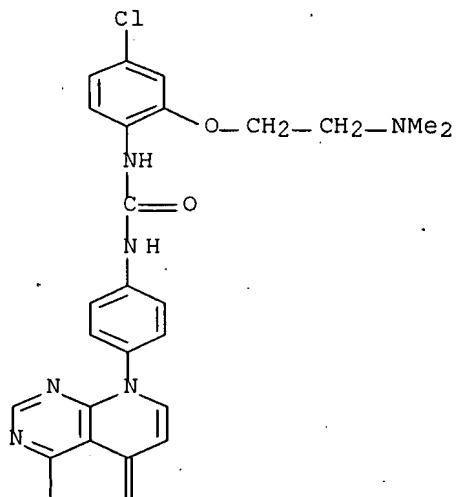
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RN 852221-96-6 HCAPLUS

CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(4-chloro-2-[2-(dimethylamino)ethoxy]phenyl)-(9CI) (CA INDEX NAME)

PAGE 1-A

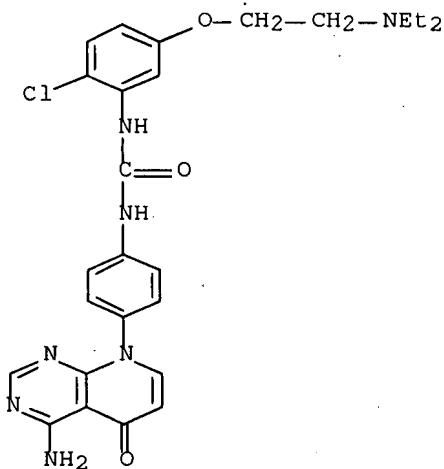


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RN 852221-98-8 HCAPLUS

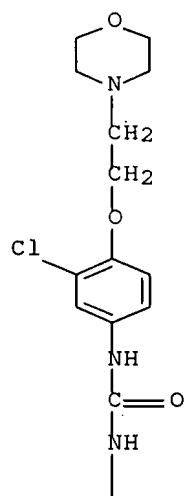
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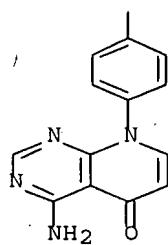
RN 866452-36-0 HCAPLUS

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L33 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:1004548 HCAPLUS Full-text

DOCUMENT NUMBER: 143:299126

TITLE: Methods for altering insulin secretion

INVENTOR(S): Lang, Florian

PATENT ASSIGNEE(S): Merck Patent GmbH, Germany

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005084651	A2	20050915	WO 2005-EP1322	200502 10
WO 2005084651	A3	20051013		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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IN 2006KN02872	A	20070608	IN 2006-KN2872	200610

PRIORITY APPLN. INFO.:

EP 2004-5404

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WO 2005-EP1322

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200502  
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ED Entered STN: 16 Sep 2005

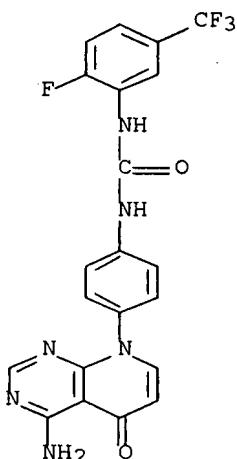
AB Modulation of the activity of glucocorticoid inducible kinase SGK1 in pancreatic islet cells restores insulin release. Also disclosed are methods and compds. useful for the treatment of glucocorticoid induced diabetes mellitus type-2.

IT 852221-35-3 852221-37-5 852221-39-7  
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 852221-47-7 852221-49-9 852221-51-3  
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 852221-94-4 852221-96-6 852221-98-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (methods for altering insulin secretion)

RN 852221-35-3 HCPLUS

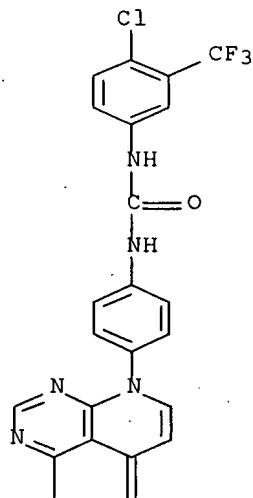
CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(2-fluoro-5-(trifluoromethyl)phenyl)-(9CI) (CA INDEX NAME)



RN 852221-37-5 HCPLUS

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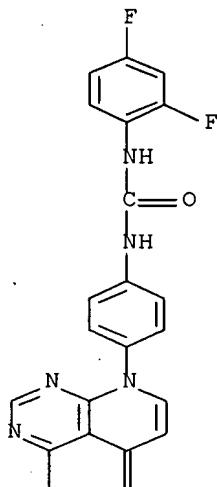
PAGE 2-A



RN 852221-39-7 HCPLUS

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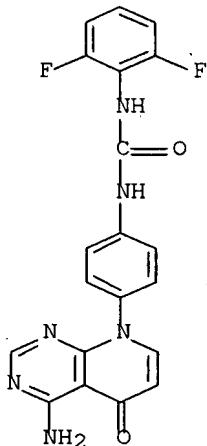
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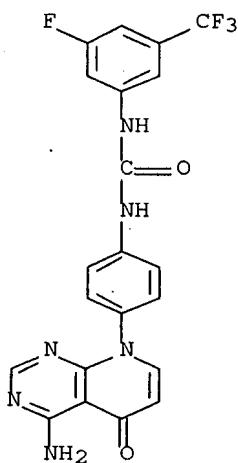
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RN 852221-43-3 HCPLUS

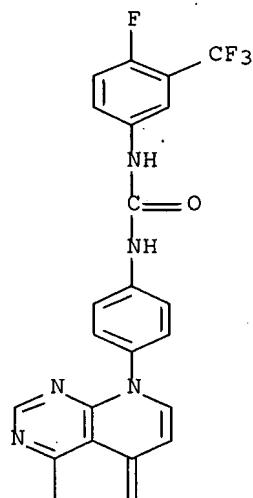
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RN 852221-45-5 HCPLUS

CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(4-fluoro-3-(trifluoromethyl)phenyl)-(9CI) (CA INDEX NAME)

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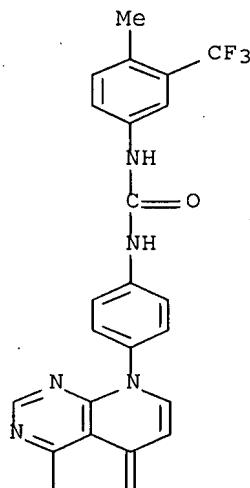
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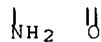
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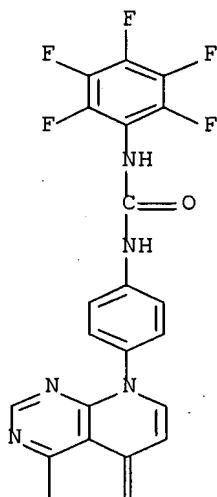
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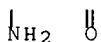
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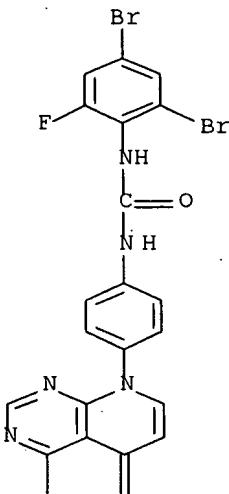
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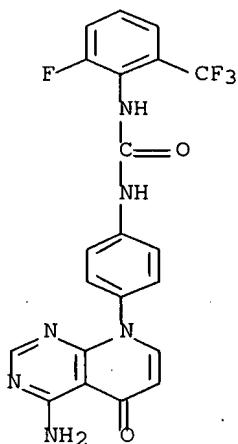


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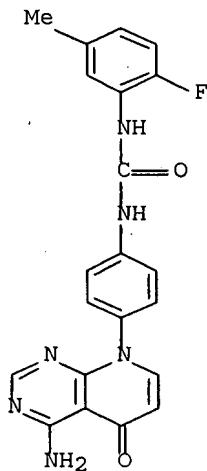
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RN 852221-55-7 HCAPLUS

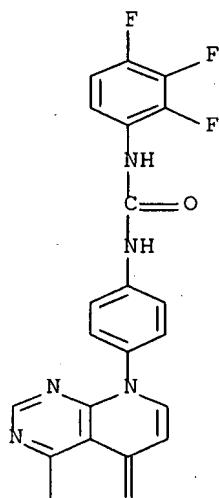
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RN 852221-57-9 HCPLUS

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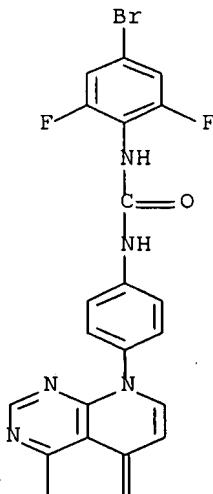
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RN 852221-59-1 HCPLUS

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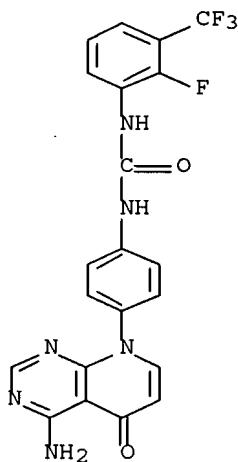


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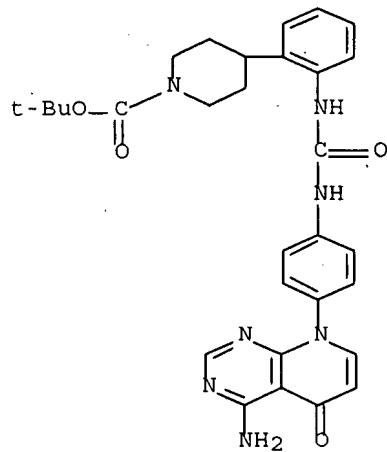
RN 852221-61-5 HCAPLUS

CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(2-fluoro-3-(trifluoromethyl)phenyl)-(9CI) (CA INDEX NAME)



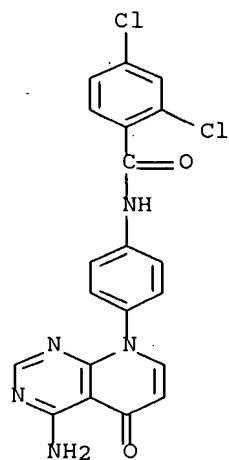
RN 852221-63-7 HCAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-[[[[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]amino]carbonyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



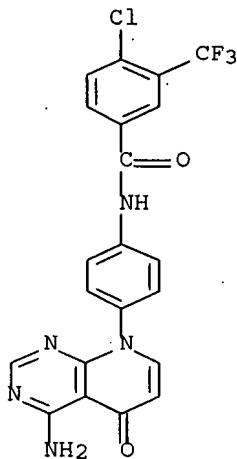
RN 852221-65-9 HCPLUS

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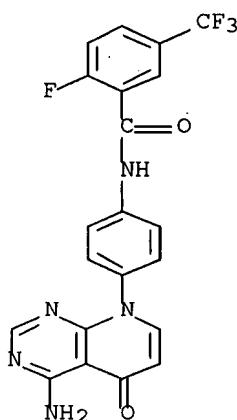
RN 852221-67-1 HCPLUS

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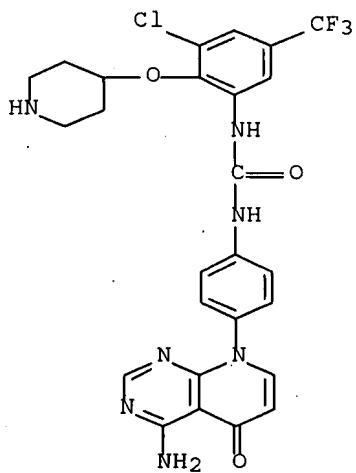
RN 852221-69-3 HCAPLUS

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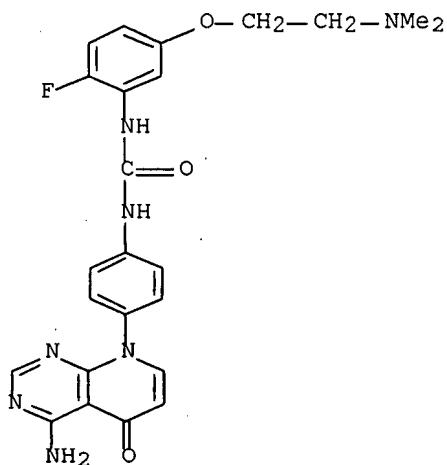
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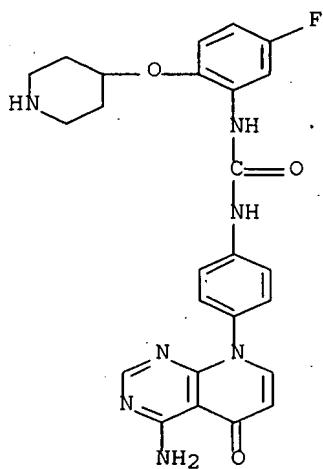
RN 852221-72-8 HCPLUS

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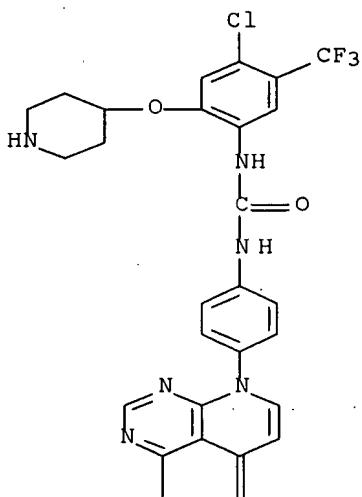
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RN 852221-76-2 HCPLUS

CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(4-chloro-2-(4-piperidinyloxy)-5-(trifluoromethyl)phenyl)- (9CI)  
(CA INDEX NAME)

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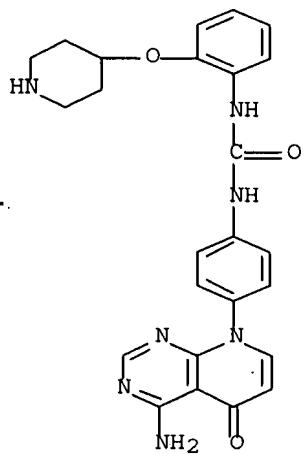


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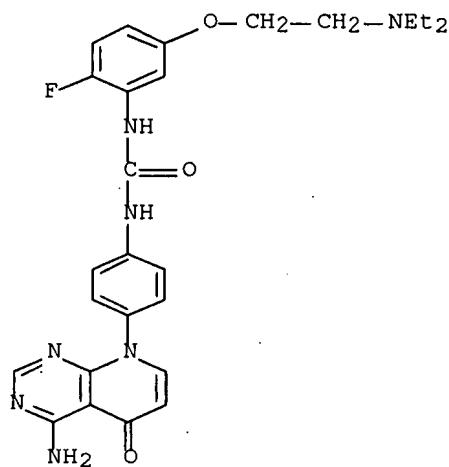
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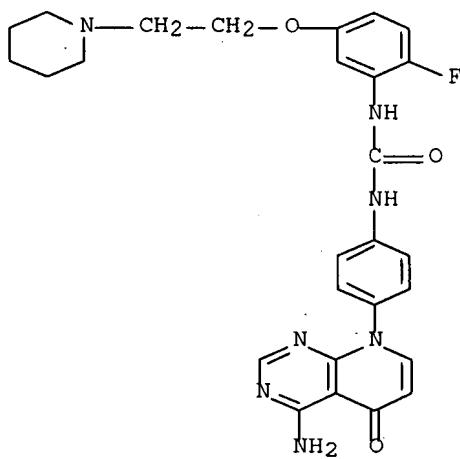
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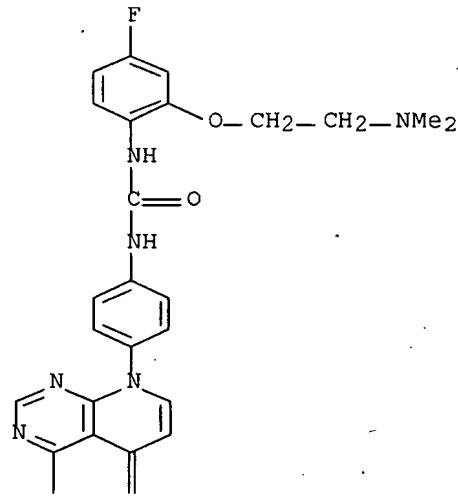
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RN 852221-84-2 HCAPLUS

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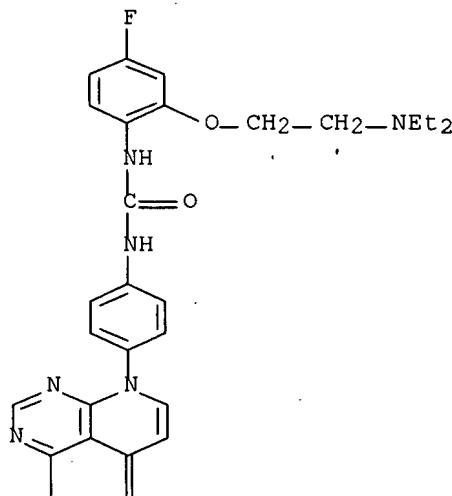
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RN 852221-86-4 HCAPLUS

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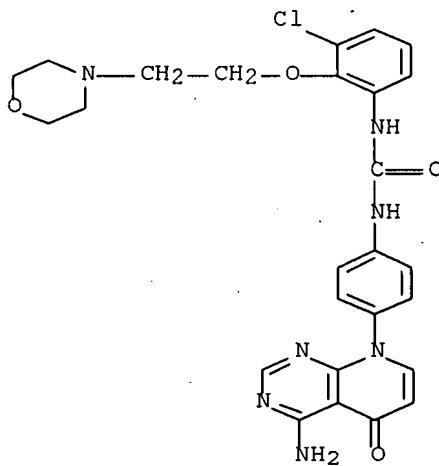


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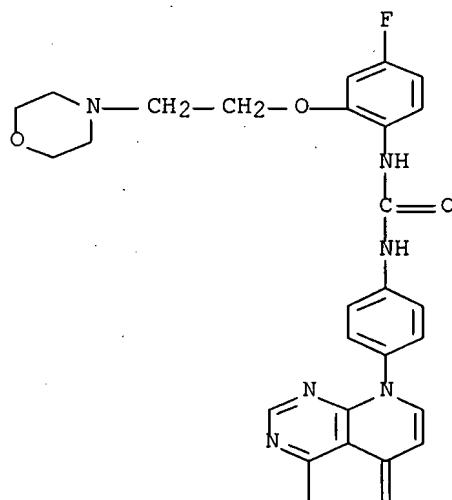
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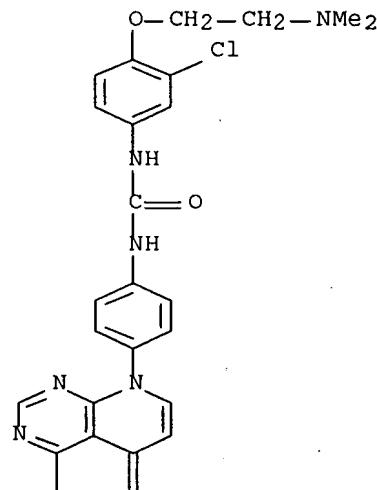
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RN 852221-92-2 HCPLUS

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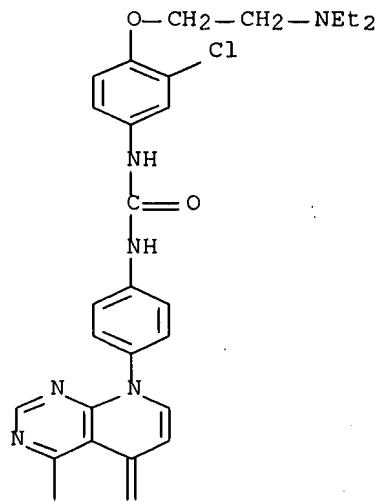
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RN 852221-94-4 HCAPLUS

CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(3-chloro-4-[2-(diethylamino)ethoxy]phenyl)- (9CI) (CA INDEX NAME)

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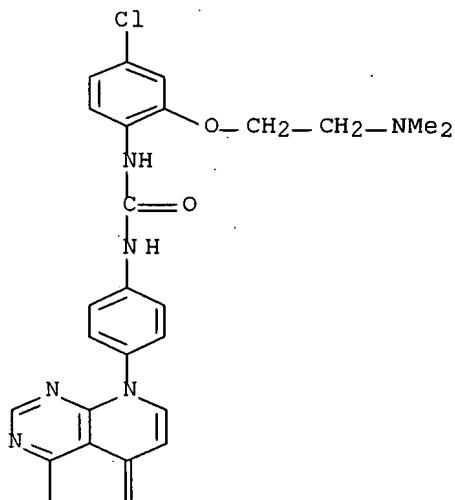
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RN 852221-96-6 HCAPLUS

CN Urea, N-[4-(4-amino-5-oxopyrido[2,3-d]pyrimidin-8(5H)-yl)phenyl]-N'-(4-chloro-2-[2-(dimethylamino)ethoxy]phenyl)- (9CI) (CA INDEX NAME)

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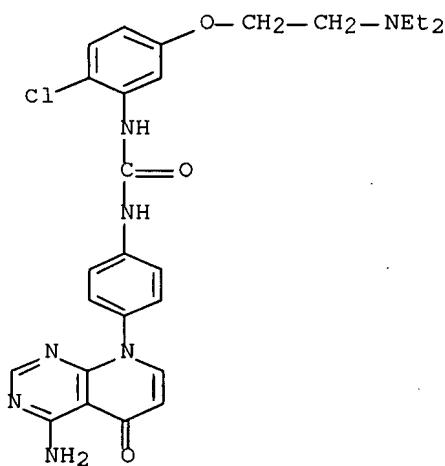


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RN 852221-98-8 HCPLUS

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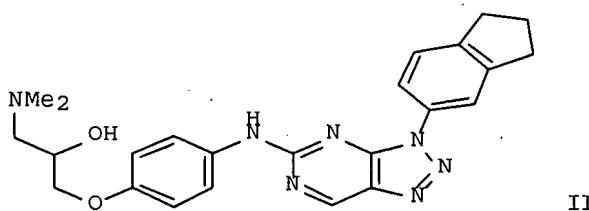
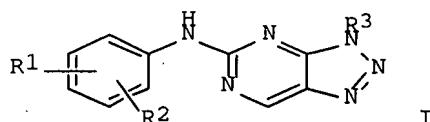
L33 ANSWER 5 OF 6 MARPAT COPYRIGHT 2007 ACS on STN

(ALL HITS ARE ITERATION INCOMPLETES)

ACCESSION NUMBER: 145:167276 MARPAT Full-text

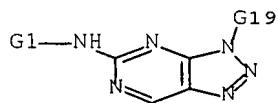
TITLE: Preparation of triazolopyrimidine derivatives as serine-tyrosine and tyrosine kinases inhibitors  
 INVENTOR(S): Ludovici, Donald W.; Connors, Richard W.; Coats, Steven J.; Liu, Li; De Corte, Bart L.; Johnson, Dana L.; Schulz, Mark J..  
 PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.  
 SOURCE: PCT Int. Appl., 97 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006076442	A2	20060720	WO 2006-US999	20060111
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2007015207	A1	20070118	US 2006-329642	20060111
PRIORITY APPLN. INFO.:			US 2005-644466P	20050114
GI				

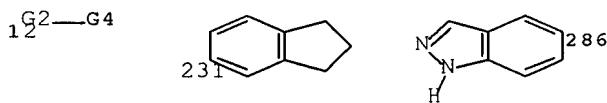


AB Title compds. represented by the formula I [wherein R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, (cyclo)alkyl, hydroxy, amino, etc.; R3 = aryl(alkyl), cycloalkyl, quinolinyl, etc.; and pharmaceutically acceptable salts thereof] were prepared as serine-tyrosine and tyrosine kinases inhibitors. For example, II was provided in a multi-step synthesis starting from reaction of 3-dimethylamino-1-propanol with 1-fluoro-4-nitrobenzene. I were tested for effects on the tyrosine kinase activity of Focal Adhesion Kinase (FAK) in vitro FAK ELISA kinase assay and CAK (Cyclin Dependent Kinase Activating Kinase) assay.

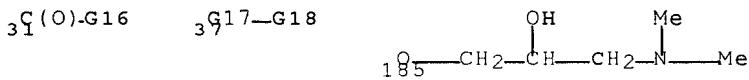
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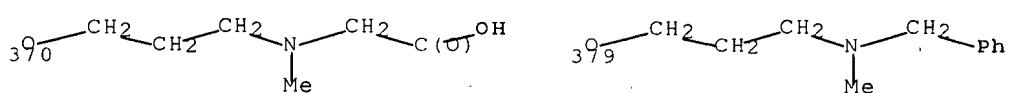
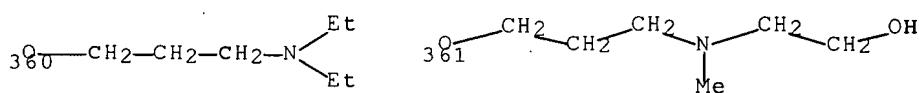
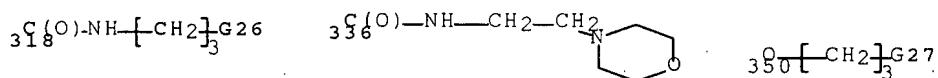
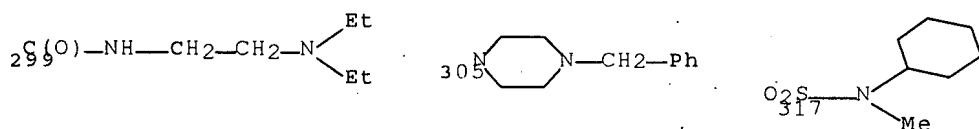
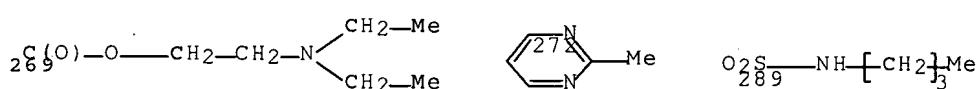
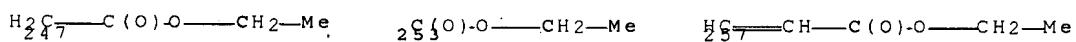
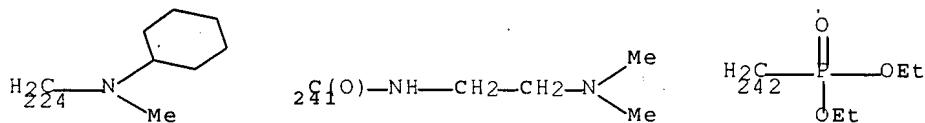
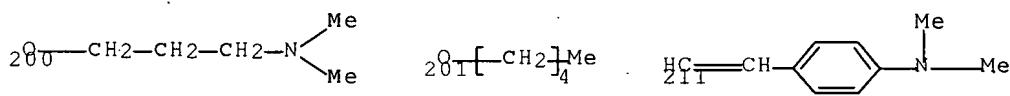


G1 = 12 / carbocycle <containing 7-11 C, aromatic, 6 normalized bonds, bicyclic, (0-1) 3-membered, (0-1) 4-membered, (0-1) 5-membered, (1-2) 6-membered, (0-1) 7-membered rings only> / heterocycle <containing 3-11 atoms, 1 or more heteroatoms, zero or more N, zero or more O, zero or more S (no other heteroatoms), aromatic, 6 or more normalized bonds, bicyclic, (0-1) 3-membered, (0-1) 4-membered, (0-1) 5-membered, (1-2) 6-membered, (0-1) 7-membered rings only> / (Specifically claimed: 231 / 286)

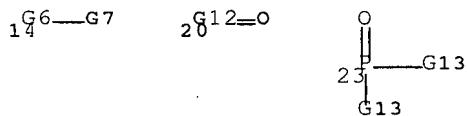


G2 = phenylene (opt. subst. by G3)  
 G3 = alkyl <containing 1-6 C> / alkoxy <containing 1-6 C> / cycloalkyl <containing 3-7 C> / OH / NH<sub>2</sub> / alkylamino <containing 1-6 C> / dialkylamino <each alkyl containing 1-6 C> / (Specifically claimed: OMe)  
 G4 = alkyl <containing 1-8 C> (opt. subst. by (1-3) G5) / alkenyl <containing 2-8 C> (opt. subst. by G14) / alkynyl <containing 2-8 C> (opt. subst. by G14) / alkoxy <containing 1-8 C> (opt. subst. by (1-3) G15) / 31 / alkoxy carbonyl <containing 1-6 C> (opt. subst. by (1-3) G15) / CONH<sub>2</sub> / alkylaminocarbonyl <containing 1-6 C> / dialkylaminocarbonyl <each alkyl containing 1-6 C> / aryl / tetrazolyl (opt. subst. by (1-3) alkyl <containing 1-6 C>) / thiadiazolyl (opt. subst. by (1-3) alkyl <containing 1-6 C>) / oxazolyl (opt. subst. by (1-3) alkyl <containing 1-6 C>) / pyrimidinyl (opt. subst. by (1-3) alkyl <containing 1-6 C>) / 37 / (Specifically claimed: 185 / 201 / 200 / 211 / 224 / 241 / Ph / 242 / 247 / 253 / 257 / CONHMe / 269 / OMe / 272 / 289 / 299 / 305 / 317 / 318 / 336 / 350 / 360 / 361 / 370 / 379)





G5 = NH2 / 14 / heterocycle <containing 1-4 heteroatoms,  
1 or more N, zero or more O, zero or more S (no other  
heteroatoms), attached through 1 or more N, monocyclic>  
(opt. subst. by (1-3) G11) / 20 / 23 /  
alkoxycarbonyl <containing 1-6 C>



G6 = NH / 16



G7 = alkyl <containing 1-6 C>  
(opt. subst. by (1-3) G8) / cycloalkyl <containing 3-7 C>  
(opt. subst. by (1-3) G8)

G8 = NH2 / alkylamino <containing 1-6 C> /  
dialkylamino <each alkyl containing 1-6 C> /  
heterocycle <containing 5-8 atoms, 1 or more heteroatoms,  
1 or more N, zero or more O, zero or more S (no other  
heteroatoms), attached through 1 or more N,  
5- to 8-membered monocyclic ring>  
(opt. subst. by (1-3) G9) / 18 / OH /  
alkoxycarbonyl <containing 1-6 C> / CO2H / aryl /  
heterocycle <containing 5-6 atoms, 1-3 heteroatoms, 1-2 N,  
0-1 O, 0-1 S (no other heteroatoms), aromatic,  
2 or more double bonds, 5- to 6-membered monocyclic ring>  
(opt. subst. by (1-3) alkyl <containing 1-6 C>)



G9 = alkyl <containing 1-6 C> /  
alkoxy <containing 1-6 C> / alkyl <containing 1-6 C>  
(subst. by 1 or more aryl) / alkoxycarbonyl <containing 1-6  
C> / CO2H / OH

G10 = heterocycle <containing 5-8 atoms,  
1 or more heteroatoms, 1 or more N, zero or more O,  
zero or more S (no other heteroatoms),  
attached through 1 or more N, 5- to 8-membered monocyclic  
ring> (opt. subst. by (1-3) G9)

G11 = alkyl <containing 1-6 C>  
(opt. subst. by 1 or more aryl) /  
alkoxycarbonyl <containing 1-6 C> / CO2H / OH

G12 = heterocycle <containing 1-4 heteroatoms,  
1 or more N, zero or more O, zero or more S (no other  
heteroatoms), attached through 1 or more N, monocyclic>  
(opt. subst. by (1-3) G11)

G13 = alkyl <containing 1-6 C>

G14 = aryl / alkoxycarbonyl <containing 1-6 C>

G15 = NH2 / 27 / heterocycle <containing 1-4 heteroatoms,  
1 or more N, zero or more O, zero or more S (no other

heteroatoms), attached through 1 or more N, monocyclic>  
(opt. substd. by (1-3) G11) / 29 / OH

$_2\text{G}^6-\text{G}^7$        $_2\text{G}^{12}=\text{O}$

G16 = NH<sub>2</sub> / 33 / heterocycle <containing 1-4 heteroatoms,  
1 or more N, zero or more O, zero or more S (no other  
heteroatoms), attached through 1 or more N, monocyclic>  
(opt. substd. by (1-3) G11) / 35 / OH

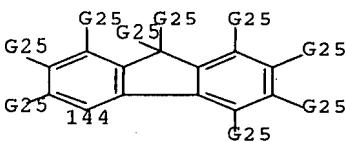
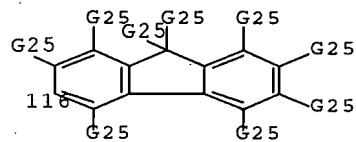
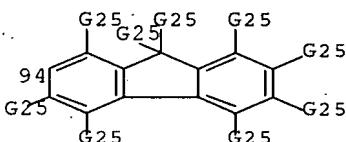
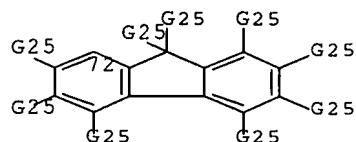
$_3\text{G}^6-\text{G}^7$        $_3\text{G}^{12}=\text{O}$

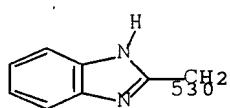
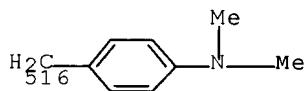
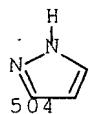
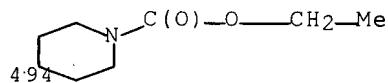
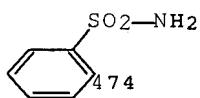
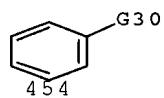
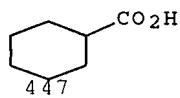
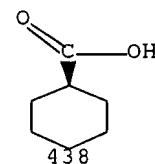
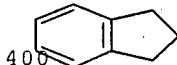
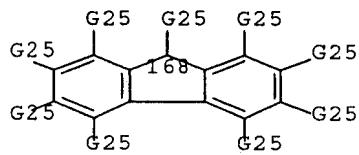
G17 = S(O) / SO<sub>2</sub>

G18 = NH<sub>2</sub> / alkylamino <containing 1-6 C> /  
dialkylamino <each alkyl containing 1-6 C> /  
heterocycle <containing 5-8 atoms, 1 or more heteroatoms,  
1 or more N, zero or more O, zero or more S (no other  
heteroatoms), attached through 1 or more N,  
5- to 8-membered monocyclic ring>  
(opt. substd. by (1-3) G9) / 39

$_3\text{G}^{10}=\text{O}$

G19 = alkyl <containing 1-6 C> (substd. by G20) /  
aryl (opt. substd. by (1-3) G21) /  
cycloalkyl <containing 3-7 C> (opt. substd. by (1-3) G22) /  
carbocycle <containing 7-11 C, aromatic, 6 normalized bonds,  
bicyclic, (0-1) 3-membered, (0-1) 4-membered,  
(0-1) 5-membered, (1-2) 6-membered,  
(0-1) 7-membered rings only> (opt. substd. by 1 or more G24)  
/ quinolinyl (opt. substd.) / benzothiazolyl (opt. substd.) /  
benzimidazolyl (opt. substd.) / pyrazolyl (opt. substd.) /  
72 / 94 / 116 / 144 / 168 / (Specifically claimed: 400 /  
Ph (opt. substd. by 1 or more G28) / cyclohexyl /  
2-naphthyl / cyclohexyl / 408 / 438 / 447 / 454 / 474 /  
CH<sub>2</sub>Ph / 494 / 504 / cyclopentyl / 516 / 530)





G20 = aryl (opt. substd. by (1-3) G21)

G21 = alkyl <containing 1-6 C> /  
alkenyl <containing 2-6 C> / alkynyl <containing 2-6 C> /  
alkoxy <containing 1-6 C> / OH / CN / F / CO2H /  
cycloalkyl <containing 3-7 C> / NH2 / 42 /  
heterocycle <containing 1-4 heteroatoms, 1 or more N,  
zero or more O, zero or more S (no other heteroatoms);  
attached through 1 or more N, monocyclic>  
(opt. substd. by (1-3) G11) / 44 / 46 /  
alkoxycarbonyl <containing 1-6 C> / 48 / pyrimidinyl /  
thiadiazolyl / tetrazolyl / pyrazolyl / oxazolyl

$_{42}^{G6}-G7$        $_{44}^{G12}=O$        $_{46}^{G(O)-G16}$        $_{48}^{G17-G18}$

G22 = OH / NH2 / 50 / heterocycle <containing 1-4  
heteroatoms, 1 or more N, zero or more O,  
zero or more S (no other heteroatoms),  
attached through 1 or more N, monocyclic>  
(opt. substd. by (1-3) G11) / 52 / 54 /  
alkoxycarbonyl <containing 1-6 C> / CO2H / 56

$_{50}^{G6}-G7$        $_{52}^{G12}=O$        $_{54}^{G(O)-G16}$        $_{56}^{G17-G23}$

G23 = NH2 / alkylamino <containing 1-6 C> /  
dialkylamino <each alkyl containing 1-6 C> /  
heterocycle <containing 5-8 atoms, 1 or more heteroatoms,  
1 or more N, zero or more O, zero or more S (no other  
heteroatoms), attached through 1 or more N,

5- to 8-membered monocyclic ring>  
 (opt. subst. by (1-3) G9) / 58 / alkyl <containing 1-6 C>

${}_{\text{5}}\text{G}^{10}=\text{O}$

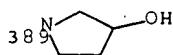
G24 = alkyl <containing 1-6 C> /  
 alkenyl <containing 2-6 C> / alkynyl <containing 2-6 C> /  
 alkoxy <containing 1-6 C> / OH / CN / F / CO<sub>2</sub>H /  
 cycloalkyl <containing 3-7 C> / NH<sub>2</sub> / 66 /  
 heterocycle <containing 1-4 heteroatoms, 1 or more N,  
 zero or more O, zero or more S (no other heteroatoms),  
 attached through 1 or more N, monocyclic>  
 (opt. subst. by (1-3) G11) / 60 / 62 /  
 alkoxycarbonyl <containing 1-6 C> / 68 / pyrimidinyl /  
 thiadiazolyl / tetrazolyl / pyrazolyl / oxazolyl

${}_{\text{6}}\text{G}^{12}=\text{O}$        ${}_{\text{6}}\text{G}^{(0)}\text{-G}^{16}$        ${}_{\text{6}}\text{G}^6-\text{G}^7$        ${}_{\text{6}}\text{G}^{17}-\text{G}^{23}$ .

G25 = H / R  
 G26 = pyrrolidino / 324 / 339 / 344



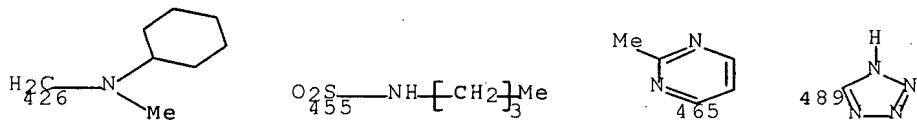
G27 = OH / morpholino / pyrrolidino / 389

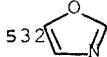


G28 = Me / OMe / F / CN  
 G29 = cyclohexyl / morpholino / 417 / 467 / 485



G30 = 426 / 455 / 465 / CONHMe / SO<sub>2</sub>NH<sub>2</sub> / 489 / 532



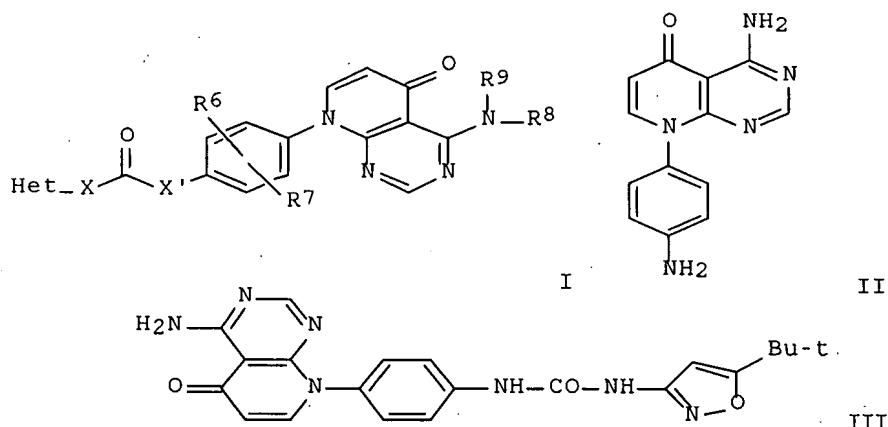


Patent location: claim 21  
 Note: or pharmaceutically acceptable salts

L33 ANSWER 6 OF 6 MARPAT COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 144:468194 MARPAT Full-text  
 TITLE: Preparation of 4-amino-pyrido[2,3-d]pyrimidin-5(1H)-ones as Raf and Tie-2 kinase inhibitors  
 INVENTOR(S): Hoelzemann, Guenter; Ackermann, Karl-August;  
 Crassier, Helene; Jonczyk, Alfred; Rautenberg,  
 Wilfried; Tarrason, Gema; Rosell-Vives,  
 Elisabet; Adan, Jaume; Cases, Claudia  
 PATENT ASSIGNEE(S): Merck Patent GmbH, Germany  
 SOURCE: Ger. Offen., 37 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

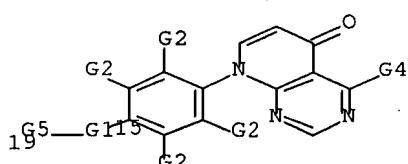
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CA 2587609	A1	20060518	CA 2005-2587609	20051020
WO 2006050800	A1	20060518	WO 2005-EP11304	20051020
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EP 1809630	A1	20070725	EP 2005-800485	20051020
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PRIORITY APPLN. INFO.:			DE 2004-10200405421520041110	
			WO 2005-EP11304	20051020

GI



AB Title compds. I [X, X' = NH with provisos; R6, R7 = H, halo, OH, etc; R8, R9 = H, A; Het = heteroarom. with 1-4 N, O, or S atoms; A = halosubstituted alkyl] and their pharmaceutically acceptable salts and formulations were prepared. For example, condensation of diamine II and 3-amino-5-tert-butylisoxazole and 4-nitrophenyl chloroformate afforded aminopyridopyrimidinone III. Compds. I are claimed to be Raf and Tie-2 kinase inhibitors (no data provided).

**MSTR 1**



G1 = C(O)

G4 = NH2

G5 = quinolinyl

Patent location:

claim 1

Note:

and pharmaceutically acceptable derivatives,

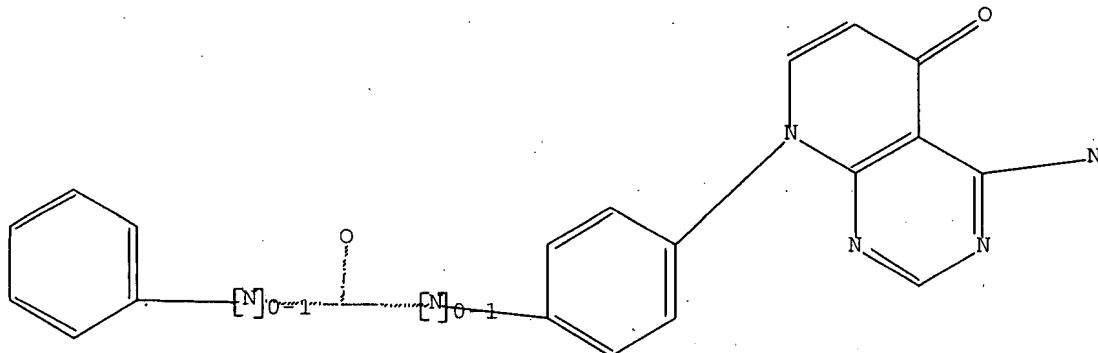
solvates, salts, and tautomers

and stereoisomers

Stereochemistry:

## SEARCH HISTORY

=> d stat que 17  
 L5 STR

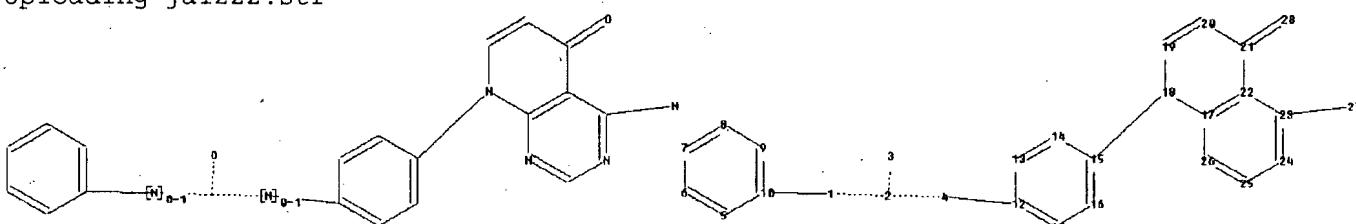


Structure attributes must be viewed using STN Express query preparation.  
 L7 66 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 1965 ITERATIONS  
 SEARCH TIME: 00.00.01

66 ANSWERS

Uploading jai222.str



chain nodes :

1 2 3 4 27 28

ring nodes :

5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26

chain bonds :

1-2 1-10 2-3 2-4 4-12 15-18 21-28 23-27

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-18

17-22 17-26 18-19 19-20 20-21 21-22 22-23 23-24 24-25 25-26

exact/norm bonds :

1-2 1-10 2-3 2-4 4-12 15-18 17-18 18-19 19-20 20-21 21-22 21-28 23-27

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 11-12 11-16 12-13 13-14 14-15 15-16 17-22

17-26 22-23 23-24 24-25 25-26

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom

=> d his nofile

(FILE 'HOME' ENTERED AT 12:41:19 ON 20 AUG 2007)

FILE 'REGISTRY' ENTERED AT 12:41:31 ON 20 AUG 2007

L5                   STRUCTURE UPLOADED  
L6                   3 SEA SSS SAM L5  
L7                   66 SEA SSS FUL L5  
                     SAV L7 JAI222/A

FILE 'HCAPLUS' ENTERED AT 16:47:27 ON 20 AUG 2007

L8                   5 SEA ABB=ON PLU=ON L7

FILE 'CASREACT' ENTERED AT 17:02:52 ON 20 AUG 2007

L9                   0 SEA ABB=ON PLU=ON L7

FILE 'REGISTRY' ENTERED AT 17:04:17 ON 20 AUG 2007

L10                  0 SEA ABB=ON PLU=ON L7 AND CASREACT/LC

FILE 'BEILSTEIN' ENTERED AT 17:06:11 ON 20 AUG 2007

L11                  0 SEA SSS SAM L5  
L12                  0 SEA SSS FUL L5

FILE 'MARPAT' ENTERED AT 17:10:13 ON 20 AUG 2007

L17                  0 SEA SSS SAM L5  
L18                  5 SEA SSS FUL L5

FILE 'HCAPLUS' ENTERED AT 17:12:39 ON 20 AUG 2007

L20                  83 SEA ABB=ON PLU=ON HOELZEMANN G?/AU  
L21                  13 SEA ABB=ON PLU=ON CRASSIER H?/AU  
L22                  200 SEA ABB=ON PLU=ON ACKERMANN K?/AU  
L23                  30 SEA ABB=ON PLU=ON STAEHLE W?/AU  
L24                  285 SEA ABB=ON PLU=ON JONCZYK A?/AU  
L25                  52 SEA ABB=ON PLU=ON RAUTENBERG W?/AU  
L26                  21 SEA ABB=ON PLU=ON MITJANS F?/AU  
L27                  12 SEA ABB=ON PLU=ON ROSELL-VIVES E?/AU  
L28                  21 SEA ABB=ON PLU=ON MITJANS F?/AU  
L29                  21 SEA ABB=ON PLU=ON ADAN J?/AU  
L30                  110 SEA ABB=ON PLU=ON SOLER R?/AU  
L31                  1 SEA ABB=ON PLU=ON L20 AND L21 AND L22 AND L23 AND L24  
                     AND L25 AND L26 AND L27 AND L28 AND L29 AND L30

FILE 'HCAPLUS' ENTERED AT 17:54:37 ON 20 AUG 2007

D QUE NOS L31  
D IBIB ED ABS L31

FILE 'REGISTRY' ENTERED AT 17:55:14 ON 20 AUG 2007

D STAT QUE L7

FILE 'HCAPLUS' ENTERED AT 17:55:35 ON 20 AUG 2007

D QUE NOS L8

FILE 'CASREACT' ENTERED AT 17:55:48 ON 20 AUG 2007

D QUE NOS L9

FILE 'MARPAT' ENTERED AT 17:56:07 ON 20 AUG 2007

D QUE NOS L18

FILE 'BEILSTEIN' ENTERED AT 17:57:06 ON 20 AUG 2007  
D STAT QUE L12

FILE 'HCAPLUS, MARPAT' ENTERED AT 17:57:23 ON 20 AUG 2007  
L32 7 DUP REM L16 L18 (3 DUPLICATES REMOVED)  
ANSWERS '1-5' FROM FILE HCAPLUS  
ANSWERS '6-7' FROM FILE MARPAT  
D QUE NOS L32  
L33 6 L32 NOT L31  
D IBIB ED ABS HITSTR 1-4  
D IBIB ABS QHIT 5-6  
D STAT QUE L7

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